Adaptive Multiscale Modeling of Large-Scale Molecular Systems

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In this work, we explore a general method of estimating modeling and computational error in very general systems and in systematically correcting error by what we call the goals algorithm [1, 2], an adaptive method that generates a sequence of models with diminishing error in some sense. The error, in our case, is in certain quantities of interest and is actually a relative error, comparing the errors in a sequence of surrogate models with the solution of a well-defined base model. Importantly, the ability to estimate and control modeling error provides a powerful framework for modeling events that take place over multiple spatial and temporal scales.

As an application of this philosophy, we consider a class of problems in molecular statics of polymers that is encountered in manufacturing nano-scale semiconductor devices. We give examples of modeling error estimation and adaptive modeling in which the sequences of surrogate models are generated using atomistic (molecular)-to-continuum scaling [3, 4, 5, 6]. Our methods provide a rigorous and systematic approach to methods of coarse-graining, dimensional reduction, homogenization, and averaging prevalent in the literature on multiscale modeling.

We also describe more recent work on extending these ideas to stochastic systems. We present new Bayesian-based approaches to calibration, validation, and uncertainty quantification of multiscale modeling, including extensions of methods of error estimates to stochastic systems.

References

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